Department of Pharmacology & Toxicology

Tuesday Seminar Series

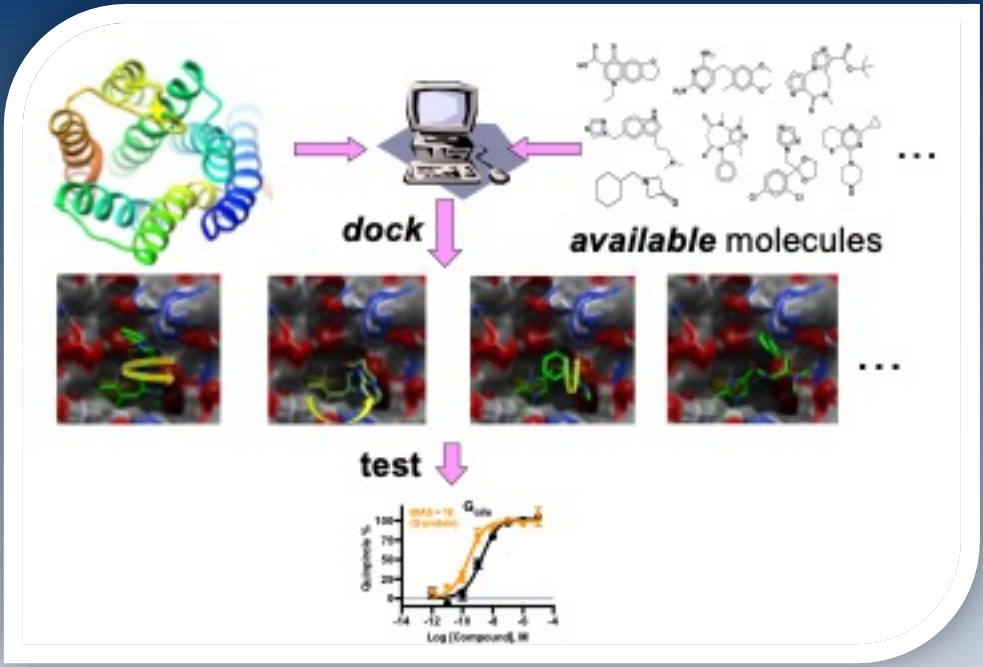
September 6th, 2022 4:00 pm MSB 4171

Ligand discovery in dark chemical space leading to biological insights

Presented by:

John Irwin Ph.D.

University of California San Francisco,
Department of Pharmaceutical Chemistry



Molecular docking is a pragmatic approach to exploit protein structure for novel ligand discovery. In the past few years, the number of molecules that can be easily docked, purchased and tested at low cost has grown from a few million to a few billion, enabling the discovery of new chemistry for new biology. This presentation will describe this approach and some of the freely available tools arising from our research. It will also show how compounds discovered using this approach have led to new understanding of the biology of the melatonin receptor and the sigma-2 receptor.

Hosted by: Matthieu Schapira

Please contact the Department directly (leonardo.salmena@utoronto.ca) if you require any accommodation(s) in order to attend this event, and we will work with you to create the appropriate arrangements.